Semiclassical approach to the line shape

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Abstract

We extend the results of Ref. [1] on one-photon electric dipole transition line shift and broadening to the case of two-photon transitions. As an example we consider the laser induced transition in antiprotonic helium produced in helium gas target. The transition is between antiprotonic helium states $(n, l) = (33, 32)$ and $(31, 30)$.

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1 Introduction

In the present paper we propose an approach to the evaluation of the density shift and broadening of the two-photon transition line profile. The foundation of our considerations is the method developed in Ref. [1] for $E1$-transitions. We slightly modify the mathematical manipulations used therein and derive close expressions for the shift of the resonance frequency and line broadening in terms of the perturbing potential mean value.

Our goal is to reduce the experimental uncertainty of recent high-precision spectroscopy measurements [2] of antiprotonic helium ($\bar{p}$He), related to the effects of the collisions of antiprotons with helium atoms. The example which we consider thoroughly is the two-photon transition from the initial $\bar{p}$He state $(n, l) = (33, 32)$ to the final state $(31, 30)$ [3]. The transition is induced by external monochromatic electromagnetic waves and is influenced by the helium gas target. Unfortunately, the available data about the $\bar{p}$He – He interaction potential [1] do not cover the whole range of interparticle distances which we are interested in. This forces us to use an extrapolation of the known potentials. Two possible extrapolations are considered and compared.

2 Two-photon transition in low density gas

The general footing of our consideration is as follows: A quantum system (emitter) is subject to a perturbation due to its randomly propagating neighbors (perturbers) and also interacts with an external electromagnetic field. The time dependent Hamiltonian of the entire system is

$$H(t) = H_0 + V(t) + W(t) \tag{1}$$

where H_0 is the unperturbed Hamiltonian of the emitter, V is the emitter–perturbers potential, and W is the electromagnetic interaction.

We suppose that the emitter possesses a full system of discrete states $\{|j>\}$ with energies $\{E_j\}$, i.e. $H_0|j>= E_j|j>$. In what follows we shall distinguish three of these states, namely the successive states $|i>, |m>$ and $|f>$ such that $E_i > E_m > E_f$. The state $|i>$ will be our initial state and $|f>$ will be the final one.

In our consideration the electromagnetic field is a superposition of two plane waves with frequencies $\omega_k, \quad k = 1, 2$. The emitter – electromagnetic

field interaction W is of the form

$$W(t) = \mathrm{w}^k cos(\omega_k t). \tag{2}$$

The coefficients w^k are emitter depending. For example, if the emitter has a dipole moment d then $\mathrm{w}^k = d.E^k$ where E^k are the electric field amplitudes. It is supposed that the frequencies ω_k are different but close to the resonance ones

$$\begin{aligned} \omega_1 &\neq \omega_2 \\ \omega_1 &\approx \omega_{mi} = (E_i - E_m)/\hbar \\ \omega_2 &\approx \omega_{fm} = (E_m - E_f)/\hbar. \end{aligned} \tag{3}$$

We make four assumptions for the potential V [1]. We suppose that, first, V it is too weak to cause quantum excitation in both emitter and perturbers. Second, the target density is low enough, so that the emitter interacts only with one perturber at a time via the pairwise emitter – perturber interaction V^0. Third, V^0 depends only on the distance R between the emitter and perturber. Forth, we adopt the Anderson approach [4] and treat the perturbers classically. Moreover, following [1], we assume that the perturber's trajectory $R(t)$ is entirely determined by the potential V^0 (plus initial conditions).

There are two important consequences of the above assumptions. First, the perturbing potential V is a sum of pairwise interactions

$$V(t) = \sum_n V^0(R_n(t)) \tag{4}$$

where n runs over all perturbers. Second, both V^0 and V have the set $\{|j>\}$ as an eigenvector system (with $\mathrm{v}_j^0(R)$ and $\mathrm{v}_j(t) = \sum_n \mathrm{v}_j^0(R_n(t))$ as eigenvalues). Therefore, these operators commute with the Hamiltonian H_0 and the evolution operator of the initial system plus perturbation is diagonal with respect to the system of states $\{|j>\}$. Its matrix elements are determined by the action over the corresponding classical solution:

$$< k|U_{H_0+V}(t_f, t_i)|j >= \delta_{kj} e^{-\frac{i}{\hbar}E_j(t_f - t_i) - i\eta_j(t_f, t_i)}. \tag{5}$$

Here

$$\eta_j(t_f, t_i)) = \frac{1}{\hbar}\int_{t_i}^{t_f} d\tau\ \mathrm{v}_j(t) \tag{6}$$

is the action of the perturbing potential when the emitter is in state $|j>$.

The matrix element of the entire system evolution operator $U(t_f, t_i)$ between states $|i>$ and $<f|$ up to the second order is

$$\begin{aligned} <f|U(t_f,t_i)|i> &= e^{-i(t_f-t_i)E_f/\hbar+i\eta_f(t_f,t_i)}[\delta_{fi} \\ &+\frac{i}{\hbar}e^{i\omega_{fi}t_i}\int_{t_i}^{t_f} d\tau\ e^{-i\omega_{fi}\tau-i\eta_{fi}(\tau,t_i)}W_{fi}(\tau) \\ &-\frac{1}{\hbar^2}e^{i\omega_{fi}t_i}\int_{t_i}^{t_f} d\tau_1\ \sum_j e^{-i\omega_{fj}\tau_1-i\eta_{fj}(\tau_1,t_i)}W_{fj}(\tau_1) \\ &\times\int_{t_i}^{\tau_1} d\tau_2\ e^{-i\omega_{ji}\tau_2-i\eta_{ji}(\tau_2,t_i)}W_{ji}(\tau_2)]. \end{aligned} \quad (7)$$

Here $\eta_{kl} = \eta_l - \eta_k$ and W_{kl} is the matrix element of the electromagnetic interaction operator W between states $< k|$ and $|l>$. We can simplify eq.(7). We can neglect the common phase factor. When $i \neq f$ we can omit the diagonal term as well. Keeping on only slowly oscillating terms we can reduce the sum over the full system of intermediate states to one term only, namely $|m><m|$. Finally, we can neglect by the same reason the first order term. As a result the evolution operator matrix element between different states $<f|$ and $|i>$ takes the form:

$$\begin{aligned} <f|U(t_f,t_i)|i> &= \frac{\mathrm{w}^2_{fm}\mathrm{w}^1_{mi}}{\hbar^2}\int_{t_i}^{t_f} d\tau_1\ e^{-i(\omega_{fm}-\omega_2)\tau_1-i\eta_{fm}(\tau_1,t_i)} \\ &\times\int_{t_i}^{\tau_1} d\tau_2\ e^{-i(\omega_{mi}-\omega_1)\tau_2-i\eta_{mi}(\tau_2,t_i)}. \end{aligned} \quad (8)$$

It is clear that the line shape, shift and broadening are determined by the double integral in eq.(8) and do not depend on the factor $\mathrm{w}^2_{fm}\mathrm{w}^1_{mi}/\hbar^2$. In what follows we shall neglect this factor and concentrate our attention on the integral which in the limit $t_i \to -\infty \quad t_f \to \infty$ we denote by U

$$U = \int dt\ e^{-i(\omega_{fm}-\omega_2)t-i\eta_{fm}(t)}I(t) \quad (9)$$

$$I(t) = \int^{t} d\tau\ e^{-i(\omega_{mi}-\omega_1)\tau-i\eta_{mi}(\tau)}. \quad (10)$$

A few remarks. What we really know is $\mathrm{v}^0_l(R)$ — the potential between the perturber and emitter in state $|l>$. With proper boundary conditions (e.g., impact parameter[1] r and velocity v) we can, using $\mathrm{v}^0_i(R)$, calculate the

[1]the distance between the emitter and the straight line which coincides with the perturber's trajectory at infinity

perturber's trajectory $R(t)$. Knowing the trajectory we can find $\mathrm{v}_l^0(t;r,v)$ but this is not enough. What we actually need is $\mathrm{v}_l(t)$ which is a result of successive random pairwise interactions. To find it we have to choose a sequence of interaction moments $\{t_i\}$ so that $V(t) = \sum_i V^0(t-t_i;r_i,v_i)$. Using $V(t)$ we have to calculate the probability of the process of interest and then to average over all possible time sequences, impact parameters and initial velocities. The task seems hopelessly complicated but before to make some simplifications let us see what we can get. We expect, on the base of our assumptions about $V(t)$, that both $\eta_{fm}(t)$ and $\eta_{mi}(t)$ are stair-like functions of time, i.e. (suppressing for a while the state indexes of η)

$$\eta(t) = \eta_0 + c_0 t + \tilde{\eta}(t). \tag{11}$$

The important term here is $c_0 t$ while $\tilde{\eta}(t)$ gives a small irregular variation around it. (The constant η_0 is irrelevant. It gives an overall phase in the transition amplitude.) Let us introduce the following simplifying notations:

$$\begin{aligned}
\underline{\omega} &= \omega_{fm} - \omega_2 + (c_0)_m - (c_0)_f && (12)\\
\omega &= \omega_{mi} - \omega_1 + (c_0)_i - (c_0)_m && (13)\\
\underline{\eta} &= \eta_m - \eta_f && (14)\\
\eta &= \eta_i - \eta_m && (15)
\end{aligned}$$

where $(c_0)_j$ is the c_0 coefficients of η_j. We will need also the Fourier transform of $\tilde{\eta}$ and $\underline{\tilde{\eta}}$

$$\tilde{\eta}(t) = \int d\xi\; e^{i\xi t}\Theta(\xi), \quad \underline{\tilde{\eta}}(t) = \int d\xi\; e^{i\xi t}\underline{\Theta}(\xi). \tag{16}$$

After regrouping the leading linear in t terms in $I(t)$, the integral takes the form

$$I(t) = \int^t d\tau e^{-i\omega\tau - i\tilde{\eta}(\tau)}. \tag{17}$$

Now, because V is small we suppose that $\tilde{\eta}(t)$ and $\underline{\tilde{\eta}}$ are small as well (see the comment below about this point), so we can make series expansion of $e^{-i\tilde{\eta}}$ and $e^{-i\underline{\tilde{\eta}}}$. Therefore, $I(t)$ and U can be rewritten as follows

$$\begin{aligned}
I(t) &= \int^t d\tau\; e^{-i\omega\tau}\,(1 - i\tilde{\eta}(\tau))\\
&= e^{-i\omega t}\left(\frac{i}{\omega} + \int d\xi\; \frac{\Theta(\xi)}{\omega - \xi} e^{i\xi t}\right) && (18)
\end{aligned}$$

$$
\begin{aligned}
U &= \int dt\; e^{-i(\underline{\omega}+\omega)t}\left(1-i\underline{\tilde{\eta}}(t)\right)\left(\frac{i}{\omega}+\int d\xi\;\frac{\Theta(\xi)}{\omega-\xi}e^{i\xi t}\right)\\
&= \int dt\; e^{-i(\underline{\omega}+\omega)t}\left(\frac{i}{\omega}+\int d\xi\left(\frac{\underline{\Theta}(\xi)}{\omega}+\frac{\Theta(\xi)}{\omega-\xi}\right)e^{i\xi t}\right)\\
&= 2\pi\left(\frac{i\delta(\underline{\omega}+\omega)}{\omega}+\frac{\underline{\Theta}(\underline{\omega}+\omega)}{\omega}-\frac{\Theta(\underline{\omega}+\omega)}{\underline{\omega}}\right). \qquad (19)
\end{aligned}
$$

The line shift Δ of the two-photon transition can be read immediately from eq.(19). Recalling the definitions of $\underline{\omega}$ and ω we see that $\underline{\omega}+\omega = (E_i - E_f)/\hbar - \omega^1 - \omega^2 + (c_0)_i - (c_0)_f$ and therefore

$$\Delta = (c_0)_i - (c_0)_f. \qquad (20)$$

Note that

$$(c_0)_l = \lim_{t\to\infty}\frac{1}{2t}\int_{-t}^{t} d\tau\; \mathrm{v}_l(\tau), \qquad (21)$$

i.e., c_0 is the mean value of the perturbing potential.

It is easy to find the line shift, but the situation with the line broadening is more complicated. At the present moment we can not say anything about it, because we do not know the explicit form of $\Theta(\xi)$ and $\underline{\Theta}(\xi)$. We shall devote the rest of the paper to show that for small but non-zero ξ the functional form of Θ (and $\underline{\Theta}$) is entirely determined by the coefficient c_0 and it is

$$\Theta(\xi) \propto \frac{c_0}{\xi}. \qquad (22)$$

We want to step back a little and comment the expansion of $e^{-i\tilde{\eta}(t)}$ used in eqs.(18,19). The assumption that $\tilde{\eta}$ is small for any t is correct, if we have a gap (or cut off) near the zero in the spectrum of $\tilde{\eta}$. The easiest may to ensure the existence of a gap is to suppose that $V(t)$ is periodic. The idea is that the mean value of the perturbing potential which determines both the shift and broadening of the line is independent, according to the Central Limit Theorem, of the assumption for periodicity, but can be easily calculated using it.

Supposing that the perturbation is periodic its period t_0 is the time between two emitter – perturber impacts. This time can be determined by the density N and temperature T of the perturbers

$$t_0 = \frac{1}{N\;\pi r_{max}^2\;\bar{v}} \qquad (23)$$

where $\bar{v} = \sqrt{8kT/\pi m}$ is the mean speed of the perturbers (m is the reduced mass of the system) and r_{max} is the distance above which we can neglect the perturbation. Obviously, r_{max} depends on V^0 but is also in our hands.

The assumption of periodicity leads to a dramatic simplification in the calculations. In the periodic picture

$$V(t) = \sum_n \bar{V}^0(t + nt_0) \tag{24}$$

where $\bar{V}_0(t)$ is the mean emitter – perturber potential

$$\begin{aligned} \bar{V}^0(t) &= \frac{1}{r_{max}^2} \int^{r_{max}} dr\ 2r \sqrt{\frac{2}{\pi}\left(\frac{m}{kT}\right)^3} \\ &\quad \times \int dv\ e^{-m\,v^2/2k\,T} v^2 V^0(t; r, v). \end{aligned} \tag{25}$$

Certainly, $\bar{V}_0(t)$ commutes with the Hamiltonian. We denote its eigenvalues with $\bar{\mathrm{v}}_l^0$. The time parameter in eq.(25) is chosen so that $t = 0$ corresponds to the apex of the perturber's trajectory. Therefore, $\bar{\mathrm{v}}_l^0(t)$ and $\mathrm{v}_l(t)$ are symmetric functions of t. For $\mathrm{v}_l(t)$ we can write down a Fourier series

$$\mathrm{v}_l(t)/\hbar = (c_0)_l + 2(c_k)_l \cos(k\omega_0 t). \tag{26}$$

$$(c_k)_l = \frac{1}{t_0\hbar} \int_{-t_0/2}^{t_0/2} dt\ \cos(n\omega_0 t)\bar{\mathrm{v}}_l^0(t). \tag{27}$$

Note that, because of the existence of r_{max}, what we really calculate is

$$(c_k)_l = \frac{1}{t_0\hbar} \int_{-t_1/2}^{t_1/2} dt\ \cos(k\omega_0 t)\bar{\mathrm{v}}_l^0(t) \tag{28}$$

where t_1 is the time for which the perturber propagates through the area of nonzero potential. According to one of our assumptions listed above $t_0 >> t_1$.

Eq.(28) is an origin of a very useful symmetry

$$\begin{aligned} t_0 &\rightarrow \alpha t_0 \\ \bar{V}^0(t) &\rightarrow \alpha \bar{V}^0(t) \end{aligned} \tag{29}$$

provided $\alpha t_0 > t_1$. Proof: Let us change t_0 so that $t_0^{new} = t_0/k$. Therefore, $\omega_0^{new} = k\omega_0$ and

$$c_n^{new} = \frac{k}{t_0\hbar} \int_{-t_1/2}^{t_1/2} \cos(nk\omega_0 t)\bar{\mathrm{v}}^0(t).dt = kc_{kn} \tag{30}$$

Coefficients c_n^{new} and c_{kn} correspond to one and the same frequency $n\omega_0^{new} = kn\omega_0$ which means that $c^{new}(\omega) = kc(\omega)$. If we rescale both t_0 and $\bar{V}^0$ as it is prescribed by eqs.(29) then we will get that $c^{new}(\omega) = c(\omega)$. Now look at eqs.(23, 25). We see that different choice of r_{max} leads exactly to the transformation (29). Increasing r_{max} we get weaker mean perturbation but it happens more often with the same gross effect. When $1/\alpha$ is not integer there will be a shift in the overtone positions, but still the Fourier coefficients will lay on one and the same curve. This curve - the envelope of the Fourier coefficients is the important one for us and it determines the line shape. Note that symmetry (29) holds both for $\alpha < 1$ and $\alpha > 1$. In the latter case the only limit on α is determine by the condition $\bar{V^0}^{new}/\hbar << 1$ no matter to what r_{max} it corresponds. We shall use such transformation to probe the line shape at small frequencies.

Using eq.(26) we get the following expressions for the actions η and $\underline{\eta}$ (see also eq.(11)):

$$\eta(t) = c_0 t + \sum_{k=1} \frac{2c_k}{k\omega_0} \sin(k\omega_0 t)) \tag{31}$$

$$\underline{\eta}(t) = \underline{c}_0 t + \sum_{k=1} \frac{2\underline{c}_k}{k\omega_0} \sin(k\omega_0 t)). \tag{32}$$

In the right hand side of the above equations all therms are small[2] but the first ones (because t is arbitrary). Therefore

$$e^{-i\eta(t)} = e^{-ic_0 t}(1 - i\frac{2c_k}{k\omega_0} \sin(k\omega_0 t)) \tag{33}$$

and

$$\begin{aligned} I(t) &= ie^{-i\omega t}\left(\frac{1}{\omega} - \frac{2c_k}{\omega^2 - (k\omega_0)^2}\cos(k\omega_0 t)\right. \\ &\left. - i\frac{2c_k\omega}{k\omega_0(\omega^2 - (k\omega_0)^2)}\sin(k\omega_0 t)\right) \end{aligned} \tag{34}$$

Now we shall need some well known formulas

$$\int_{-\infty}^{\infty} dt\; e^{-i\omega t}\cos(\bar{\omega}t) = \pi\left(\delta(\omega + \bar{\omega}) + \delta(\omega - \bar{\omega})\right) \tag{35}$$

$$\int_{-\infty}^{\infty} dt\; e^{-i\omega t}\sin(\bar{\omega}t) = i\pi\left(\delta(\omega + \bar{\omega}) - \delta(\omega - \bar{\omega})\right) \tag{36}$$

[2]this gives another way to determine the maximal α (or the minimal ω_0) we can use

Using these equations we obtain that U (up to a phase) is

$$\begin{aligned} U &= 2\pi \left(\frac{1}{\omega}\delta(\underline{\omega}+\omega) + \right. \\ &+ \left(\frac{c_k}{\underline{\omega}(\underline{\omega}+\omega)} - \frac{\underline{c}_k}{\omega(\underline{\omega}+\omega)} \right) \delta(\underline{\omega}+\omega-k\omega_0) + \\ &+ \left. \left(\frac{c_k}{\underline{\omega}(\underline{\omega}+\omega)} - \frac{\underline{c}_k}{\omega(\underline{\omega}+\omega)} \right) \delta(\underline{\omega}+\omega+k\omega_0) \right) \end{aligned} \tag{37}$$

Hereafter we suppose that one of the frequencies ω^k, say ω^1, is fixed. Then the probability interpretation of eq.(37) is exactly the same as for the simple one-photon transition amplitude between unperturbed states. The only difference is that instead of one line now we have a bunch of closely separated lines with intensities proportional to the square of the coefficients in front the delta functions. In practice, where the real potential is not periodic, we see the envelope of these lines. This is in agreement with eqs.(28,29) according to which at the limit $t_0 \to \infty$ the inter line distance ω_0 is so small that the Fourier coefficients c_k form a line. The important moment is that the Fourier coefficients calculated for any t_0 lay on this line. Therefore, we can fix t_0, find the Fourier coefficients $\{c_k\}$ and $\{\underline{c}_k\}$ and interpolate them with functions $c(\xi)$ and $\underline{c}(\xi)$.

The expression for U given in eq.(37) is very close to that in eq.(19). It is clear that the line shift again is determined by eq.(20) but now we can say something more about line shape. The envelope functions $c(\xi)$ and $\underline{c}(\xi)$, according to eq.(28), behave like constants for $\xi \to 0$. So, we can smoothly continue them for negative ξ making them symmetric with respect to $\xi = 0$. As a result U for sufficiently small but non zero ξ is (see also eq.(22))

$$U \propto \frac{1}{(\underline{\omega}+\omega)} \left(\frac{c_0}{\underline{\omega}} - \frac{\underline{c}_0}{\omega} \right) \tag{38}$$

Eq.(38) allows us to estimate for given ω^1 the line broadening σ (calculated as the difference between frequencies for which the probability is half of its maximum)

$$\sigma = \sqrt{(\omega \pm \sqrt{2}\underline{c}_0)^2 \pm 4\sqrt{2}c_0\omega}. \tag{39}$$

The choice of the sign in eq.(39) depends on which of discriminants is positive. If both discriminants are positive then we have double line. (The

doublet can be seen easily as one much broader line in experiments with non monochromatic light sources.)

The dependence of the Fourier coefficients c on density N can be read from eqs.(23,28)

$$c_k(N) = \left(\frac{c_k(N_0)}{N_0}\right) N. \tag{40}$$

As a consequence of eq.(40) the line shift and broadening also depend on N

$$\Delta(N) = \left(\frac{c_0(N_0) + \underline{c}_0(N_0)}{N_0}\right) N \tag{41}$$

$$\sigma(N) = \left(\frac{\sqrt{2}|\underline{c}_0(N_0)|}{N_0}\right) N \quad \text{if } |\underline{c}_0|,\ |c_0| >> |\omega| \tag{42}$$

$$\sigma(N) = |\omega| \quad \text{if } |\underline{c}_0|,\ |c_0| << |\omega|. \tag{43}$$

3 Numerical results

The system we consider [3] consists of antiprotonic helium as emitter and the helium atoms in a gas target as perturbers. The initial, final and intermediate states are $|i >= (33, 32)$, $|f >= (31, 30)$ and $|m >= (32, 31)$ respectively. The target is at $p = 1$ mbar and $T = 6^{\circ}$K.

We use two sets of perturbing potentials $\{\mathrm{v}_i^0, \mathrm{v}_m^0$ and $\mathrm{v}_f^0\}$ corresponding to two different extrapolations of the data we have about the potential energy surface (PES) for the $\bar{p}$He – He interaction. The results obtained from the first set of potentials will be indicated by prime and those obtained from the second set by double prime.

The double integral in Eq. (25) was calculated as a left Riemann sum over a regular set of $N = 1000$ points for the impact parameter $r \leq r_{max} = 25$ a.u. and using a Gauss-type quadrature formula with $M = 6$ points for the average over the Maxwell distribution for the velocity.

We obtain the following values for the coefficients c_0 and $\underline{c}_0$ needed to estimate the line shift and broadening according to eqs.(41 – 43)

$$c_0'(N_0)/N_0 = 5.2\ \ 10^{-13}[\text{Hz cm}^3] \tag{44}$$

$$\underline{c}_0'(N_0)/N_0 = 4.8\ \ 10^{-13}[\text{Hz cm}^3] \tag{45}$$

$$c_0''(N_0)/N_0 = 1.4\ \ 10^{-12}[\text{Hz cm}^3] \tag{46}$$

$$\underline{c}_0''(N_0)/N_0 = 1.4\ \ 10^{-12}[\text{Hz cm}^3]. \tag{47}$$

This gives that the line shift is

$$\Delta'(N_0)/N_0 = 1.0\ \ 10^{-12}[\text{Hz cm}^3] \quad (48)$$
$$\Delta''(N_0)/N_0 = 2.8\ \ 10^{-12}[\text{Hz cm}^3]. \quad (49)$$

We can use eq. (42) to obtain the line broadening when $|\omega_1| \approx |\omega_{mi} + c_0|$, i.e., when we have a fine tuning between the first laser frequency and the inter level distance between the initial and intermediate states. Then the result is

$$\sigma'(N_0)/N_0 = 6.8\ \ 10^{-13}[\text{Hz cm}^3] \quad (50)$$
$$\sigma''(N_0)/N_0 = 2.0\ \ 10^{-12}[\text{Hz cm}^3]. \quad (51)$$

Eq.(43) describes the off-resonance situation. In this case the line broadening does not depend on the target density

$$\sigma(N) = |\omega_{mi} - \omega_1| \quad \text{if} \ \ |\omega_{mi} - \omega_1| >> |\underline{c}_0|,\ |c_0|. \quad (52)$$

In every other case the general formula (39) for the line broadening has to be used.

The discrepancy between results for the two approximating sets of potentials is about a factor of three. This indicates that the PES extrapolation we have used in the construction of the potentials is not reliable. The problem could be solved only by extending the PES to shorter distances between the antiproton and He^+ ion, corresponding to the average radius of the antiproton orbit in $\bar{p}$He in states with $n \sim 30$.

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